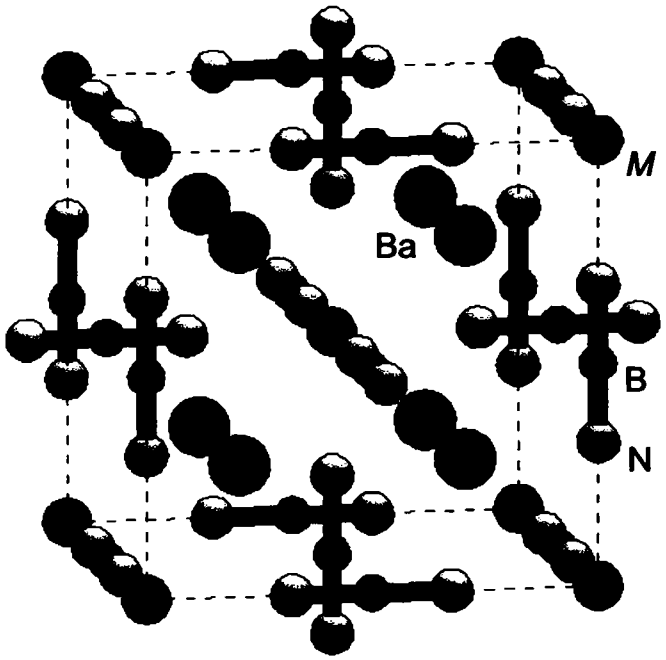
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Crystal structures of strontium octabarium hexakis(dinitridoborate) and europium octabarium hexakis(dinitridoborate), MBa$_8$[BN$_2$]$_6$ (M = Sr, Eu)

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M = Sr, Eu

Abstract

B$_6$Ba$_8$N$_{12}$Sr, cubic, $Im\bar{3}m$ (no. 229), a = 7.913(1) Å, V = 495.6 Å^3, Z = 1, $R_{gt}(F)$ = 0.031, $wR_{ref}(F^2)$ = 0.098, T = 293 K.

B$_6$Ba$_8$EuN$_{12}$, cubic, $Im\bar{3}m$ (no. 229), a = 7.839(1) Å, V = 481.8 Å^3, Z = 1, $R_{gt}(F)$ = 0.014, $wR_{ref}(F^2)$ = 0.056, T = 293 K.

Source of material

The title compounds MBa$_8$[BN$_2$]$_6$ (M = Sr, Eu) were synthesized from the binaries Sr$_2$N (EuN), Ba$_2$N and hexagonal BN (molar ratios 2-3 : 8 : 6) in arc-welded niobium ampoules at 1375 K. The reaction products are pale yellow (M = Sr) and black (M = Eu) crystalline powders, respectively, which are sensitive to air and moisture.

Discussion

The cubic title structures are isotypic to that of NaBa$_4$[BN$_2$]$_3$ (= ½ Na$_2$Ba$_8$[BN$_2$]$_6$) [1,2] in which the Na$^+$ ions in the 2a position are replaced by the bivalent Sr^{2+} and Eu^{2+}, respectively, being randomly distributed. Because of the electroneutrality, the occupancy of the 2a site is 50 %. Characteristic structural units are discrete linear [N–B–N]$^{3-}$ anions with d(B—N) = 1.335(9) Å (M = Sr) and 1.335(7) Å (M = Eu). The unusual black color was already reported for Eu$_3$[BN$_2$]$_2$ which contains solely Eu(II), as confirmed by Mößbauer spectroscopy and magnetic measurements [3,4].

1. Strontium octabarium hexakis(dinitridoborate), SrBa$_8$[BN$_2$]$_6$

Table 1. Data collection and handling.

Crystal:	pale yellow plate, size 0.10 × 0.20 × 0.25 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	731.91 cm^{-1}
Diffractometer, scan mode:	Siemens P2$_1$, $\omega/2\theta$
$2\theta_{max}$:	55.08°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	359, 78
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 71
$N(param)_{refined}$:	11
Programs:	SHELXS-97 [5], SHELXL-97 [6], ATOMS [7]

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Sr(1)	2a	0.53(2)	0	0	0	0.015(1)	U_{11}	U_{11}	0	0	0
Ba(1)	8c		¼	¼	¼	0.0375(8)	U_{11}	U_{11}	0.0062(2)	$-U_{12}$	$-U_{12}$
B(1)	6b		0	0	½	0.014(5)	U_{11}	0.035(9)	0	0	0
N(1)	12e		0.331(1)	0	0	0.026(4)	0.034(3)	U_{22}	0	0	0

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2. Europium octabarium hexakis(dinitridoborate), $EuBa_8[BN_2]_6$

Table 3. Data collection and handling.

Crystal:	black plate, size 0.07 × 0.15 × 0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	771.10 cm^{-1}
Diffractometer, scan mode:	Siemens $P2_1$, $\omega/2\theta$
$2\theta_{max}$:	55.06°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	347, 76
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma(I_{obs})$, 74
$N(param)_{refined}$:	11
Programs.	SHELXS-97 [5], SHELXL-97 [6], ATOMS [7]

Table 4. Atomic coordinates and displacement parameters (in $Å^2$).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Eu	2*a*	0.503(6)	0	0	0	0.0210(5)	U_{11}	U_{11}	0	0	0
Ba	8*c*		¼	¼	¼	0.0429(4)	U_{11}	U_{11}	0.0052(1)	$-U_{12}$	$-U_{12}$
B	6*b*		0	0	½	0.027(4)	U_{11}	0.036(6)	0	0	0
N	12*e*		0.3298(8)	0	0	0.040(4)	0.049(2)	U_{22}	0	0	0

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